Fate Report for Case # P-19-0140

Fate Summary Statement

Fate Summary Statement: P-19-0140
FATE:
[redacted] with MP < 25 °C (E)
log Kow = 4.50 (E)
S = 6.56 mg/L at 25 °C (E)
VP = [redacted] torr at [redacted] °C (M)
BP = [redacted] °C (M)
H = 1.79E-2 (E)
log Koc = 2.67 (E)
log Fish BCF = 2.64 (440) (E)
log Fish BAF = 3.38 (2,400) (E)
POTW removal (%) = 50-90 via possible sorption and stripping; OECD 310(Headspace):
0.3%/28d NRB.
Time for complete ultimate aerobic biodeg > mo
Sorption to soils/sediments = low - moderate
Volatilization half-life from a standard river = 2 hrs
Volatilization half-life from a standard lake = 7 da
Atmospheric Oxidation Half-life = 97 hr via OH radical
Atmospheric Oxidation Half-life = 490 hr via ozone
PBT Potential: P3BU
FATE: Migration to ground water = moderate – rapid

Analogue found (include identifier and database)

Relevant Structure(s)
Water Parent
Landfill Parent
Air / Incineration Parent
Parent % incineration 99.9% (hazardous waste incinerator)

Environmental Fate Determination

PMN #: P-19-0140
Summary: The new chemical substance is estimated to be very persistent in the environment and its bioaccumulation potential is unknown. Thus, it is unknown whether repeated exposures will cause food-chain effects via accumulation in exposed organisms.

Fate: Environmental fate is the determination of which environmental compartment(s) a chemical moves to, the expected residence time in the environmental compartment(s) and removal and degradation processes. Environmental fate is an important factor in determining exposure and thus in

determining whether a chemical may present an unreasonable risk. EPA estimated physical/chemical and fate properties of the new chemical substance using data for analogue(s) (highly fluorinated aliphatic chemicals), data submitted for the new chemical substance, and EPI (Estimation Program Interface) Suite™ (http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface). In wastewater treatment, the new chemical substance is expected to be removed with an efficiency of 50% to 90% due to stripping and possible sorption. Removal of the new chemical substance by biodegradation is negligible. Sorption of the new chemical substance to sludge, soil, and sediment is expected to be low to moderate. Migration of the new chemical substance to groundwater is expected to be moderate to rapid due to low to moderate sorption to soil and sediment. Due to moderate reported vapor pressure, the new chemical substance is expected to undergo moderate volatilization to air. Overall, these estimates indicate that the new chemical substance has moderate potential to volatilize to air and has moderate to high potential to migrate to groundwater.

Persistence : Persistence is relevant to whether a new chemical substance is likely to present an unreasonable risk because chemicals that are not degraded in the environment at rates that prevent substantial buildup in the environment, and thus increase potential for exposure, may present a risk if the substance presents a hazard to human health or the environment. EPA estimated degradation half-lives of the new chemical substance using data for analogue(s) (highly fluorinated aliphatic chemicals) and data submitted for the new chemical substance. EPA estimated that the new chemical substance's aerobic and anaerobic biodegradation half-lives are > 6 months. These estimates indicate that the new chemical substance may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation : Bioaccumulation is relevant to whether a new chemical substance is likely to present an unreasonable risk because substances that bioaccumulate in aquatic and/or terrestrial species pose the potential for elevated exposures to humans and other organisms via food chains. EPA estimated that the new chemical substance has unknown bioaccumulation potential based on uncertainty about bioaccumulation of the new chemical substance. The new chemical substance is estimated to be very persistent in the environment and its bioaccumulation potential is unknown. Thus, it is unknown whether repeated exposures will cause food-chain effects via accumulation in exposed organisms.

[redacted]
Fate Assessor: Card, Marcella
SMILES: [redacted]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[redacted]	[redacted]
Molecular Wt.:	[redacted]	[redacted] g/mol
% < 500:		

Property	Measured/Calculated Value	EPI
% < 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:					NaN °C (Exp.) -65.33000183105469 °C (Est., Joback) -71.07168579101562 °C (Est., Gold) -68.20083618164062 °C (Est., Selected)
Boiling Point:	73.5				NaN °C (Exp.) 72.94 °C (Est.) 346.1009216308594 °K (Est.)
BP Pressure:	760.0				
Vapor Pressure:	108.0				NaN mmHg (Exp.) 17407.138431518553 Pa (Est., Antoine) 130.56463623046875 mmHg (Est., Antoine) 16572.619547720118 Pa (Est., Grain) 124.30521255096772 mmHg (Est., Grain) 17718.11184888768 Pa (Est., Mackay) 132.89713512314304 mmHg (Est., Mackay) 16989.878989619338 Pa (Est., Selected) 127.43492439071824 mmHg (Est., Selected) NaN Pa (Est., SubCooled) NaN mmHg (Est., SubCooled)
Water Solubility:			0.0066		NaN (Exp.) 0.905242919921875 (Est.)
Log P:			4.5		
Log Kow:					NaN (Exp.) 4.5 (Est.)
Log Koc:	NaN				6.153030553846979 (Est., log(MCI)) 7.241731553111513 (Est., log(Kow)) 470.1400146484375 L/kg (Est., MCI) 1396.510009765625 L/kg (Est., Kow)
Log BCF:					3.16 L/kg wet-wt

Property	Measured Value	Method	Estimated Value	Method	EPI
Henry's Law:					NaN atm-m3/mole (Exp.) 0.01789850927889347 atm-m3/mole (Est., Bond) 0.0 atm-m3/mole (Est., Group)

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):		**Volatilization (t1/2) - River (hr):**		**Volatilization (t1/2) - Lake (da):**	
Atm Ox Potential (t1/2)OH (hr):	8.076571794022694	**Atm Ox Potential (t1/2)O3 (hr):**	0.0560000017285347	**Atm Ox Potential(t1/2) Total (hr):**	
MITI Linear:	0.10000000149011612	**MITI NonLinear:**	0.0		
Biodeg Linear:	-1.5	**Biodeg NonLinear:**	0.0		
Biodeg Survey ult:	1.2999999523162842	**Biodeg Survey Prim:**	2.5999999046325684		
STP (% removal) Total:	91.39601391219422%	**STP (% removal) Biodeg:**	0.18776511135574145%		
STP (% removal) Ads:	37.88274830106909%	**STP (% removal) Air:**	53.325500940885746%		

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic	

Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	
Persistence - Air:	
Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
3	U	2 (HH, ECO)	

Exposure-Based Testing

Exposure-Based Testing:	

Fate Ratings

Removal in WWT/POTW (Overall):

Removal in WWT/POTW (Overall):	50-90

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	1-2	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	3	Extensive	Moderate	Low	Negligible	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Biodegradation Removal:	4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	3-4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	3-4	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments:

Bio Comments:	Fate Study Summaries are available. Fish log BAF = 3.38 (2,400). The fugacity spreadsheet and the EPI output file for the PMN material are attached.

Fate Comments:

Fate Comments:	OECD 310(Headspace): 0.3%/28d NRB.

Comments/Telephone Log

Artifact	Update/Upload Time

Artifact	Update/Upload Time
[redacted]	[redacted]